C.442. COMPLEXITY IN EXPERIMENTAL DESIGN II. COMPARING SECOND- ORDER DESIGNS

Keywords: Design complexity; A and D efficiency; subset efficincy; small second-order designs

1. INTRODUCTION

Given a model $Y=f(X)\beta+\varepsilon$ with design matrix X, the design is often evaluated using estimative criteria such as A, D or E efficiency (cf. Kiefer (1959), Fedorov (1972)) and information functionals (Pukelsheim (1980)), or using predictive criteria such as G efficiency (Kiefer (1959)) and the integrated prediction variance (Box and Draper (1959)). Part I of this study considers complexity (van Emden (1971)) as a further criterion used elsewhere in model selection (Maklad and Nichols (1980)). It is seen that complexity gages the nonorthogonality of X through the ellipticity of $\Sigma=[f(X)'f(X)]^{-1}$, and thereby the degree of regularity of confidence ellipsoids for β. In particular, complexity is related directly to A-efficiency, and inversely to D-efficiency. In Part II we now apply these concepts in a comparative evaluation of selected second-order designs in current usage.

A partial list includes the central composite designs (CCD's) of Box and Wilson (1951), the small composite designs (SCD's) of Hartley (1959), the designs (BBD's) of Box and Behnken (1960), the minimal designs (BDD's) of Box and Draper (1974), the hybrid designs $H310$ and $H311B$ of Roquemore (1976), the designs (HOD's) of Hoke (1974), the designs (NOD's) of Notz (1982), and others. Properties of these designs have been reported in the literature.

To fix ideas, consider a second-order model

$$\{Y_i=\beta_0+\sum_{r=1}^{k}\beta_r X_{ir}+\sum_{r=1}^{k}\beta_{rr}X_{ir}^2+\sum_{r<s}\beta_{rs}X_{ir}X_{is}+\varepsilon_i;i=1,\ldots,n\} \quad (1.1)$$

in $k=3$ regressors $\{X_{i1},X_{i2},X_{i3}\}$ having $p=1+k(k+3)/2=10$ parameters given as $\beta'=[\beta_0,\beta_1,\beta_2,\beta_3,\beta_{11},\beta_{22},\beta_{33},\beta_{12},\beta_{13},\beta_{23}]$. These are partitioned subsequently as $\beta=[\beta_0',\beta_L',\beta_Q',\beta_I']'$, where $\beta_L'=[\beta_1,\beta_2,\beta_3]$,

$\beta'_Q = [\beta_{11}, \beta_{22}, \beta_{33}]$, and $\beta'_I = [\beta_{12}, \beta_{13}, \beta_{23}]$ respectively comprise the linear, the pure quadratic, and the interaction coefficients of the model. We next compare designs for models of this type.

2. COMPARING DESIGNS FOR β

Of eight designs cited with $k = 3$, all are unsaturated on adding a center run as necessary; all have been scaled to $\sqrt{3}$ at the design perimeter; and the *SCD* and *CCD* have axial points at $\alpha = \sqrt{3} = 1.732$. To compare designs under the model (1.1), let $V(\hat{\beta})/\sigma^2 = \Lambda$ with eigenvalues $\lambda = [\lambda_1, \dots, \lambda_k]'$. The relevant diagnostics are the arithmetic ($\bar{\lambda}$) and geometric ($GM(\lambda)$) means of λ, the complexity coefficient $\phi(\Lambda)$ of van Emden (1971), the ellipticity coefficient $C_0(\Lambda) = (1/k)\ \mathrm{tr}(\Lambda)/|\Lambda|^{1/k}$, and the trace ($\mathrm{tr}(\Lambda)$) and determinant ($|\Lambda|$) of Λ. The latter determine the *A* and *D* efficiencies for each design, whereas complexity gages regularity of confidence ellipsoids for β as noted. However, since $\bar{\lambda} = \mathrm{tr}(\Lambda)/10$, and since $\phi(\Lambda)$ and $C_0(\Lambda)$ are related one-to-one, as are $GM(\lambda)$ and $|\Lambda|$, it suffices to report only $C_0(\Lambda)$, $\mathrm{tr}(\Lambda)$ and $20GM(\lambda)$ as equivalent gages of complexity (van Emden (1971)) and the *A* and *D* efficiencies for each design. The scaling $20GM(\lambda)$ is chosen for convenience. These appear in columns 2–4 of Table I for each of the eight designs, as they pertain to complexity and efficiency for the full parameters β.

We prefer $C_0(\Lambda)$ and $GM(\lambda)$ to $\phi(\Lambda)$ and $|\Lambda|$. For if designs X and Z, with $\Sigma = [f(X)'f(X)]^{-1}$ and $\Omega = [f(Z)'f(Z)]^{-1}$, are of equal complexity, *i.e.*, $C_0(\Sigma) = C_0(\Omega)$, then their comparative *A* and *D* efficiencies are identical as gaged by $C_A(X)/C_A(Z)$ and $C_D(X)/C_D(Z)$, with $C_A(X) = \mathrm{tr}(\Sigma)$ and $C_D(X) = |\Sigma|^{1/k}$, and similarly for $C_A(Z)$ and $C_D(Z)$.

From Table I designs *BBD* and *CCD* stand out for their greater *A* and *D* efficiencies in comparison with other designs. Designs *H*310 and *CCD* have comparable *A*-efficiencies, but their complexities and *D*-efficiencies are related inversely as shown in Theorem 1 of Part I. The designs *NOD*, *HOD*, and *BDD* are less *A* and *D* efficient than the remaining designs, although their complexities are roughly comparable. Further such comparisons are supported by Table I, and a summary is provided in Section 4.

TABLE I Diagnostics based on dispersion matrices $V(\hat{\beta})/\sigma^2$ for the full parameters and $V(\hat{\beta}_L)/\sigma^2$ for the linear coefficients of eight small designs

Design	*Coefficients* β			*Coefficients* β_L		
	$C_0(\Lambda)$	$tr(\Lambda)$	$20GM(\lambda)$	$C_0(\Lambda)$	$tr(\Lambda)$	$20GM(\lambda)$
*H*310	1.3256	1.9873	2.9983	1.0000	0.3565	2.3764
*H*311*B*	1.8743	2.4000	2.5610	1.0000	0.3000	2.0000
SCD	2.0976	3.2278	3.0775	1.0000	0.5000	3.3333
BBD	1.9602	2.1667	2.2107	1.0000	0.2500	1.6667
CCD	2.1953	2.0575	1.8745	1.0000	0.2144	1.4286
NOD	2.0930	4.2500	4.0613	1.0000	0.3750	2.5000
HOD	1.8873	4.4023	4.6652	1.2157	0.6973	3.8238
BDD	1.4383	3.1906	4.4367	1.0000	0.4764	3.1762

3. COMPARISONS FOR SUBSETS OF PARAMETERS

3.1. Background

Special features of a response surface are often germane. Linear coefficients determine slopes at the origin, whereas second-order coefficients determine the shapes and orientations of its contours. Moreover, the signs and magnitudes of interaction coefficients quantify the presence and degree of synergistic or antagonistic effects between pairs of variables, as in studies of the efficacy of drugs in combination. For further discussion see Heady (1952), Heady and Dillon (1961), Myers (1971), Wardrop and Myers (1990), and Myers and Montgomery (1995), for example. Since different uses entail different features, it is essential to compare designs on these issues.

These needs embody the concept of local design efficiencies for subsets of parameters, including A_S, D_S, G_S and other local criteria as in Atwood (1969), Kiefer (1961), Sibson (1974), and Wardrop and Myers (1990), for example. Here we add local complexity to that list, and we accordingly compare these designs with reference to β_L, β_Q, and β_I along the lines of the comparisons for β as given in Table I.

3.2. Linear Coefficients

Diagnostics for the linear coefficients β_L are reported in the last three columns of Table I. The designs $\{SCD, HOD, BDD\}$ are comparatively inefficient for β_L under both A_S and D_S efficiencies. The *HOD* has complexity of 1.25, in comparison with the value 1.00 for the other designs. Confidence ellipsolids for β_L for the latter designs are all spherical owing to regularity of the designs.

3.3. Quadratic Coefficients

Diagnostics for the pure quadratic coefficients β_Q are reported in the first four columns of Table II. The designs $\{NOD, HOD, BDD\}$ are especially A_S and D_S inefficient for β_Q. Moreover, all designs have complexities greater than 1. Further trends are summarized in Section 4.

3.4. Interaction Coefficients

Diagnostics for the interaction coefficients β_I appear in the last three columns of Table II. The *SCD* is especially D_S-inefficient and somewhat A_S-inefficient, followed by *BDD*, *H*311*B*, and *HOD*. In practice these would be avoided in studies of synergism and antagonism, in favour of designs $\{BBD, CCD, NOD\}$. The *HOD* has complexity of 1.24, in comparison with values at or near 1.00 for the other designs. Further trends are summarized in the section following.

TABLE II Diagnostics based on dispersion matrices $V(\hat{\beta}_Q)/\sigma^2$ for the quadratic coefficients and $V(\hat{\beta}_I)/\sigma^2$ for the interaction coefficients of eight small designs

Design	*Coefficients* β_Q			*Coefficients* β_L		
	$C_0(\Lambda)$	$tr(\Lambda)$	$20GM(\lambda)$	$C_0(\Lambda)$	$tr(\Lambda)$	$20GM(\lambda)$
*H*310	1.0302	0.6429	4.1605	1.0000	0.4831	3.2209
*H*311*B*	1.4163	0.5000	2.3536	1.0000	0.6000	3.9999
SCD	1.5283	0.4778	2.0842	1.0000	1.2500	8.3333
BBD	1.1814	0.5833	3.2917	1.0000	0.3333	2.2222
CCD	1.5110	0.4683	2.0660	1.0000	0.3750	2.5000
NOD	1.1218	2.6250	15.6006	1.0000	0.3750	2.5000
HOD	1.2493	2.4785	13.2263	1.2402	0.7266	3.9055
BDD	1.0546	1.5712	9.9325	1.0012	0.6781	4.5150

4. CONCLUSIONS

A recurring problem is to choose among the many second-order designs now available using appropriate criteria. The approach taken here features the regularity of confidence ellipsoids for the parameters, placing yet another tool in the hands of prospective users. A summary of our findings follows, where the grouping and ordering $\{D_1, D_2\} \succ \{D_3\}$ is meant to convey the idea that designs D_1 and D_2 are roughly comparable, each being more efficient than design D_3. Regarding complexity, $\{D_1\} \prec \{D_2, D_3\}$ conveys that D_1 is less complex than D_2 and D_3, which are roughly comparable in complexity. With these conventions we may summarize our principal findings as follows.

Efficiencies and complexities for the full parameters β satisfy

- A-efficiency: $\{H310,\ H311B,\ SCD,\ BBD,\ CCD\} \succ \{NOD,\ HOD,\ BDD\}$.
- D_S-efficiency: $\{BBD,\ CCD\} \succ \{H310,\ H311B,\ SCD\} \succ \{NOD,\ HOD,\ BDD\}$.
- Complexity: $\{H310,\ BDD\} \prec \{H311B,\ BBD,\ HOD\} \prec \{SCD,\ CCD,\ NOD\}$.

Efficiencies and complexities for the linear coefficients β_L satisfy

- A_S-efficiency: $\{BBD,\ CCD\} \succ \{H310,\ H311B,\ NOD\} \succ \{SCD,\ HOD,\ BDD\}$.
- D_S-efficiency: $\{BBD,\ CCD\} \succ \{H310,\ H311B,\ NOD\} \succ \{SCD,\ HOD,\ \mathrm{BDD}\}$.
- Complexity: All designs have $C_0(\Lambda) = 1.00$ except HOD with $C_0(\Lambda) = 1.22$.

Efficiencies and complexities for the pure quadratic coefficients β_Q satisfy

- A_S-efficiency: $\{H310,\ H311B,\ SCD,\ BBD,\ CCD\} \succ \{NOD,\ HOD,\ BDD\}$.
- D_S-efficiency: $\{H311B,\ SCD,\ CCD\} \succ \{H310,\ BBD\} \succ \{NOD,\ HOD,\ BDD\}$.
- Complexity: $\{H310,\ BDD\} \prec \{BBD,\ NOD,\ HOD\} \prec \{H311B,\ SCD,\ CCD\}$.

Efficiencies and complexities for the interaction coefficients β_I satisfy

- A_S-efficiency: $\{H310,\ H311B,\ BBD,\ CCD,\ NOD\} \succ \{SCD, HOD, BDD\}$.
- D_S-efficiency: $\{BBD,\ CCD,\ NOD\} \succ \{H310,\ H311B,\ HOD,\ BDD\} \succ \{SCD\}$.
- Complexity: All disigns have $C_0(\Lambda)$ near 1.00 except HOD with $C_0(\Lambda) = 1.24$.

In summary, a synthesis of our findings suggests that the designs may be grouped as $\{H310, H311B, BBD,\ CCD\} \succ \{SCD,\ NOD,\ HOD,\ BDD\}$ in terms of overall efficiency. Comparisons of their complexities are less clear, except that designs $H310$ and BDD appear least complex overall in comparison with the other designs.

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C.443. CAN THE IDEA OF THE QH TEST FOR NORMALITY BE USED FOR TESTING THE WEIBULL DISTRIBUTION?

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Shapiro and Wilk (1965) introduced a statistic W for testing the hypothesis that a set of data was a random sample from a normal distribution. The W test statistic is a ratio of two estimators of the distribution scale parameter; one of which is a proper estimator independent of the null hypothesis and the other only provides a proper estimator if the null hypothesis is true. The test statistic was denoted by

$$W = \frac{b^2}{S^2},$$

where b is a linear estimator of the scale parameter using generalized least square regression of the order statistics on their expected values, and S^2 is the usual symmetric estimator of the scale parameter up to a constant. This idea was extended to test the hypothesis for the exponential distribution in Shapiro and Wilk (1972), generalized for the normal distribution by Shapiro and Francia (1972) by substituting the identity matrix for the covariance matrix and this was later adapted to